STABILITY OF IMPURITIES WITH COULOMB POTENTIAL IN GRAPHENE WITH HOMOGENEOUS MAGNETIC FIELD

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Dedicated to Elliott H. Lieb on the occasion of his 80th birthday

Abstract. Given a 2-dimensional no-pair Weyl operator W_Z with a point nucleus of charge Z, we show that a homogeneous magnetic field does not lower the critical charge beyond which it collapses.

1. Introduction

Perfect graphene is modeled in continuum one-particle approximation by a two-dimensional free Weyl operator (massless Dirac operator). Non-perfect graphene has additional potentials; a particular case of importance is the presence of an impurity of Coulomb type (see the review of Castro Neto et al. [3]). As opposed to non-relativistic mechanics, in relativistic mechanics both kinetic energy and the Coulomb potential energy have the same linear scaling for large momenta which implies the existence of a critical coupling constant. This explains the interest in the subject in the physics literature, see, e.g., Pereira et al. [15] and Shyvtov et al. [17]. The critical coupling constant as occurring in these papers can be mathematically thought of as that coupling constant were a natural definition of self-adjointness ceases to exist. In addition to the electric impurity potential it is often also important to study the systems with an additional homogeneous magnetic field perpendicular to the graphene sheet. Of course, the question arises to what extend the presence of the magnetic field changes the critical coupling constant.

If one is interested in multi-particle effects it is essential to have a well defined multi-particle Hamiltonian (see [5] and the references therein). Because of the Weyl operator's unboundedness from above and below, a naive addition of the one-particle operators acting on the various particles plus their interactions – as would be natural in non-relativistic quantum mechanics – does not give meaningful Hamiltonians (Brown and Ravenhall [2]). This problem can – on a physical level – be overcome by a quantum field theoretical treatment. Approximately, one can use the no-pair Hamiltonians initially introduced by Brown and Ravenhall [2] and further developed by Sucher [18]. Because a non-perturbative analytic treatment of quantum electrodynamics is not available, we will concentrate on the second alternative.

A description of – one-particle – no-pair operators in an nutshell is as follows: the state space on which the no-pair Hamiltonians are defined depend on a Dirac sea in a similar way as the Fock representation of the electron-positron field depends on the initial splitting of the Hilbert space into electron and positron space (see Thaller [20, Section 10.1.1]). The Dirac sea is defined through an orthogonal projection $(1 - \Lambda)$ in the state space of the Weyl operator W_Z, i.e., the Hilbert space $L^2(\mathbb{C}^2, \mathbb{R}^2)$. The projection Λ is assumed fixed. The physically allowed states of Dirac particles will be those which are orthogonal to the sea, i.e., they are eigenstates of Λ. Metaphorically speaking the physical states are the vapor above the

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Dirac sea. The no-pair approximation will then be the Weyl operator projected onto the states of fixed particle number N – in our case $N = 1$ – in the vapor, i.e., $B_z := \Lambda W_Z \Lambda$.

It is reasonable to expect that expectations of the no-pair Hamiltonians B_Z are bounded from below if Z is small (close to zero) and is unbounded from below for large Z. The critical coupling Z_c constant is the value of the coupling constant where this change of behavior occurs. A priori Z_c can be expected to depend on the choice of the Dirac sea. A particular simple choice is to take the Dirac sea as the one defined by the Weyl operator with the external homogeneous field. It is exactly this operator which we will be interested in. Our goal is to show that Z_c does not depend on the presence of a homogeneous magnetic field.

Although the rest of the paper is on the one-particle level, our interest in the one-particle stability stems from the multi-particle stability: the multi-particle energy of the no-pair Hamiltonian is bounded from below if and only if the corresponding one-particle Hamiltonian is bounded from below (see [5]).

Our contribution is organized as follows: to escape the inconclusiveness of heuristic arguments, we give a precise mathematical formulation of the problem, collect some well known relevant facts and state our result (Section 2). To prepare for the proof we study the partial wave analysis of underlying energy form in Section 3. In Section 4 we give the actual proof of our claim. The appendices contain auxiliary material which we collect for the convenience of the reader.

2. Notation, Formulation of the Problem, and Main Result

The Weyl operator (massless Dirac operator) of a particle of charge $-e$ in two dimensions in a magnetic field $\partial_1 A_2 - \partial_2 A_1$ with vector potential $\mathfrak{A} := (A_1, A_2)$ and an electric potential φ is given by

$$W_{\mathfrak{A},\varphi} := v\boldsymbol{\sigma} \cdot (\mathfrak{p} + \frac{e}{c}\mathfrak{A}) - e\varphi \tag{1}$$

where v, c, and e are positive constants. Depending on the application, v could be, e.g., the velocity of light or the Fermi velocity in graphene, c is the velocity of light, and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ are the first two Pauli matrices, i.e.,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}.$$

In this paper we are mainly interested in the case of a homogeneous magnetic field of strength $B > 0$ orthogonal to the x_1-x_2-plane, i.e., $\mathfrak{A}(x) = \frac{B}{2}(-x_2, x_1)$, and an electric field generated by a nucleus of atomic number Z, i.e., $\varphi(x) = Ze/|x|$. (Note that $B < 0$ corresponds just to a reflection of the coordinates $x \to -x$. For $B = 0$ see Remark 6 of Section 2.) This operator is to be self-adjointly realized in $L^2(\mathbb{R}^2, \mathbb{C}^2)$. Following Brown and Ravenhall [2] – see also Sucher [18, 19] – we will project these operators to the orthogonal space of a Dirac sea. More precisely, we are interested in the quadratic form of $W_{\mathfrak{A},\varphi}$ restricted to the positive spectral subspace

$$\mathfrak{H} := \{\psi \in L^2(\mathbb{R}^2, \mathbb{C}^2) \mid \psi = \Lambda\psi\}$$

with $\Lambda := \chi_{(0,\infty)}(W_{\mathfrak{A},0})$.

By dilation $W_{\mathfrak{A},\varphi}$ is unitarily equivalent to $\sqrt{eB/(2c\hbar)}vW_{e^2Z/(\hbar v)}$. Thus it suffices to study $W_Z := \boldsymbol{\sigma} \cdot (\mathfrak{p} + (-x_2, x_1)) - \frac{Z}{|x|}$ assuming that $e = v = \hbar = 1$. We use complex notation $z := x_1 + \mathrm{i}x_2$, and, correspondingly $\bar\partial := \frac{1}{2}(\partial_1 + \mathrm{i}\partial_2)$ and $\partial := \frac{1}{2}(\partial_1 - \mathrm{i}\partial_2)$ and introduce $d := -2\mathrm{i}(\partial + \bar z/2)$ and $d^* := 2\mathrm{i}(-\bar\partial + z/2)$. This

allows us to write more compactly

$$W_Z = \begin{pmatrix} 0 & d \\ d^* & 0 \end{pmatrix} - \frac{Z}{|\cdot|}. \tag{2}$$

We define $\mathfrak{q}_0$ as the linear span of the functions $\phi_{m,n}$ defined in (36) of the Appendix. We also define $\mathfrak{Q}_0$ as the linear span of the spinors $\psi_{m,n}$ defined in (44) of the Appendix.

Theorem 1. *The quadratic form $(\psi, W_Z\psi)$ is positive on $\mathfrak{Q}_0$ and extends to a closed form $\mathcal{E}$ on $\mathfrak{Q}$ which is bounded from below, if*

$$Z \leq Z_c := \left(\frac{\Gamma(\frac{1}{4})^4}{8\pi^2} + \frac{8\pi^2}{\Gamma(\frac{1}{4})^4} \right)^{-1}. \tag{3}$$

For $Z > Z_c$ the form is unbounded from below.

We remark:

(1) Physically $\mathcal{E}[\psi]$ is the energy of an electron in the state ψ on top of the Fermi sea defined by $\mathfrak{H}^\perp$ in the quantum dot defined by the homogeneous magnetic field and an interstitial atom with charge Z.
(2) If $Z \leq Z_c$, then the form $\mathcal{E}$ defines – according to Friedrichs [9, Satz 3] – a unique positive self-adjoint operator whose form domain includes $\mathfrak{q}_0$ and extends ΛW_z. It is called the no-pair Hamiltonian of one electron in the quantum dot.
(3) For scalar type magnetic operators, like Schrödinger operators $(\mathfrak{p}-\mathfrak{A})^2+V$ or Chandrasekhar operators $|\mathfrak{p}-\mathfrak{A}|+V$, it is known that $\mathfrak{A}$ does not lower the ground state energy because of the diamagnetic inequality. For operators involving spin in an essential way like the Pauli operator this is known to be false. Although, in our case, we cannot expect the energy to increase when $\mathfrak{A}$ is turned on, our result shows, that the energy is not lowered dramatically, i.e., the critical coupling constant is not lowered. Thus, the boundedness result can be interpreted as a weak form of the diamagnetic inequality.
(4) The result for $Z > Z_c$ means physically that the electron is pulled into the nucleus of the interstitial atom as the trial function of the proof will indicate.
(5) The critical coupling constant in the three dimensional non-magnetic case with arbitrary non-negative mass was found by Evans et al [6]. Tix [21, 22] sharpened the result to strict positivity with a lower bound linear in the mass.
(6) The critical coupling constant in the 2-dimensional non-magnetic case was investigated by Bouzouina [1]. An error in the constant he obtained was corrected by Walter [23].
(7) The 3-dimensional magnetic case – for a rather big class of magnetic fields – was treated by Matte and Stockmeyer [14]. They showed that the critical constant is not lowered by an intricate resolvent method. The generality of their result is paid for by the absence of an explicit lower bound on the energy. The bonus of our direct approach based on Lieb and Yau's [13] strategy in the variant found in [6] – compared to transfering the methods of [14] – is our result on the positivity of the energy.
(8) The numerical value of the critical coupling constant is $Z_c \approx 0.3780$ which is compared with the expected critical coupling constant $\tilde{Z}_c$ of the existence of a distinguished self-adjoint extension of the non-magnetic Weyl operator W_Z. Pereira et al [15] and Shytov et al [17] suggest in physical language

and using physical arguments that $\tilde{Z}_c = 1/2$. Recently Warmt [24, Satz 2.2.6] showed that this is indeed the case.

3. The positive spectral subspace and partial wave analysis

The fact, that we are dealing with spinors in the positive spectral subspace of W_0 allows us to reduce the problem to unrestricted scalar wave functions (see [8, Section 1.1] for the three dimensional case).

Lemma 1. *The map*

$$\begin{aligned} \Phi : L^2(\mathbb{R}^2) &\to \mathfrak{H} \\ u &\mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} u \\ d^*|d^*|^{-1}u \end{pmatrix} \end{aligned} \tag{4}$$

is unitary.

Furthermore, its restriction to $\mathfrak{q}_0$ is a unitary map from $\mathfrak{q}_0$ to $\mathfrak{Q}_0$ with the associated scalar products.

Proof. First, we remark that Φ maps indeed to $\mathfrak{H}$. This holds, since $\mathfrak{H}$ is the closure of $\mathfrak{Q}_0$ in the L^2-norm.

To show that Φ is surjective, assume $\psi = (u, v)^t \in \mathfrak{H}$ and orthogonal to

$$\{(w, d^*|d^*|^{-1}w)^t | w \in L^2(\mathbb{R}^2)\}.$$

This implies

$$(u, w) + (|d^*|^{-1}dv, w) = (u + |d^*|^{-1}dv, w) = 0$$

for all $w \in L^2(\mathbb{R}^2)$, i.e., $u = -|d^*|^{-1}dv$.

Next we remark that

$$\begin{pmatrix} -|d^*|^{-1}d\phi_{m,n} \\ \phi_{m,n} \end{pmatrix}$$

$n \in \mathbb{N}_0$, $m \in \mathbb{Z}$ are eigenvectors with negative eigenvalue, namely $-2\sqrt{n + m_+ + 1}$. Thus

$$\left(\begin{pmatrix} -|d^*|^{-1}dv \\ v \end{pmatrix}, \begin{pmatrix} \phi_{m,n} \\ -d^*|d^*|^{-1}\phi_{m,n} \end{pmatrix} \right) = 0$$

for all n and m which implies $(|d^*|^{-1}dv, \phi_{m,n}) = 0$, i.e., $dv = 0$. Therefore, $\psi = (0, v)^t$. Such vectors are in the kernel of W_0, i.e., orthogonal to the positive spectral space, so that in the end $\psi = 0$ is the only vector in the positive spectral space which is orthogonal to $\Phi(L^2(\mathbb{R}^2, \mathbb{C}^2))$.

The identity $(u, v)_{L^2(\mathbb{R}^2)} = (\Phi u, \Phi v)_{\mathfrak{H}}$ for all $u, v \in L^2(\mathbb{R})$ is immediate, as is the unitarity of the restriction. □

Using Lemma 1 we define the operator $w_Z := \Phi^* W_Z \Phi$ on $\mathfrak{q}_0$. The associated quadratic form on $\mathfrak{q}_0$ is

$$(u, w_Z u) := (u, \Phi^* W_Z \Phi u) = (u, |d^*|u) - Z(u, Vu) \tag{5}$$

with

$$V = \frac{1}{2} \left(\frac{1}{|\cdot|} + |d^*|^{-1} d \frac{1}{|\cdot|} d^* |d^*|^{-1} \right). \tag{6}$$

Corollary 1. *The operators ΛW_Z on $\mathfrak{Q}_0$ and w_z on $\mathfrak{q}_0$ are unitarily equivalent by Lemma 1. In particular both operators and also the associated forms have all the same lower maximal bound.*

Next we calculate the matrix elements of w_Z in the orthonormal basis given by the eigenfunctions $\phi_{m,n}$ of w_0. First of all, we remark that this matrix is diagonal in the angular momentum quantum number m. We get for the matrix t^m associated with w_0 the following matrix elements

$$t^m_{n,n'} := (\phi_{m,n}, w_0\phi_{m,n'})\delta_{n,n'} = 2\sqrt{n+m_++1}\delta_{n,n'} \tag{7}$$

which is immediate from the eigenvalues equation (45); for the first summand of the potential V (see (6)) we get the matrix $v^{m,0}$ with matrix elements

$$\begin{aligned} v^{m,0}_{n,n'} =&(\phi_{m,n}, \frac{1}{|\cdot|}\phi_{m,n'}) \\ =&\frac{1}{\pi\sqrt{(n+1)_{|m|}(n'+1)_{|m|}}} \sum_{k=0}^{\min\{n,n'\}} \frac{(k+1)_{|m|-\frac{1}{2}}}{(n-k+\frac{1}{2})_{\frac{1}{2}}(n'-k+\frac{1}{2})_{\frac{1}{2}}} \end{aligned} \tag{8}$$

which is obtained by explicit calculation using the generating function of the generalized Laguerre polynomials [12, Formula 22.9.15] and their recursion relations [12, Formula 6.1.15]. (For convenience we use Pochhammer's notation $(z)_a := \Gamma(z+a)/\Gamma(z)$ [see also (49)].) Eventually, the second summand of the potential V yields the matrix $v^{m,1}$ with matrix elements

$$v^{m,1}_{n,n'} = (d^*|d^*|^{-1}\phi_{m,n}, \frac{1}{|\cdot|}d^*|d^*|^{-1}\phi_{m,n'}) = \begin{cases} v^{m+1,0}_{n,n'} & \text{if } m \geq 0 \\ v^{m+1,0}_{n+1,n'+1} & \text{if } m < 0. \end{cases} \tag{9}$$

This can be obtained from (8) by observing that

$$d^*|d^*|^{-1}\phi_{m,n} = \begin{cases} \mathrm{i}\phi_{m+1,n} & \text{if } m \geq 0, \\ -\mathrm{i}\phi_{m+1,n+1} & \text{if } m < 0. \end{cases} \tag{10}$$

Thus, the quadratic form $\mathcal{E}_m$ of the matrix $(\phi_{m,n}, w_Z\phi_{m,n'})$, for fixed angular momentum $m \in \mathbb{Z}$, on $l^2_0(\mathbb{N}_0)$ – the subscript denotes sequences of compact support – is given as

$$\mathcal{E}_m[a] = \sum_{n,n'=0}^{\infty} \overline{a_n}\left[t^m_{n,n'} - \tfrac{Z}{2}(v^{m,0}_{n,n'} + v^{m,1}_{n,n'})\right] a_{n'}. \tag{11}$$

As mentioned in Appendix A, $(\phi_{m,n}, w_Z\phi_{m',n'}) = (\phi_{m,n}, w_Z\phi_{m,n'})\delta_{m,m'}$, i.e., both, potential and kinetic energy, are diagonal in m. Thus,

$$(u, w_z u) = \sum_{m\in\mathbb{Z}} \mathcal{E}_m[a^m] \tag{12}$$

where we write $a^m_n := (\phi_{m,n}, u)$ for the generalized Fourier coefficients for $u \in \mathfrak{q}_0$ and where we collect those coefficients with the same angular momentum quantum number m and write

$$a^m = (a^m_0, a^m_1, \ldots). \tag{13}$$

Obviously, $(a^m_n)_{n\in\mathbb{N}_0,\ m\in\mathbb{Z}} \in l^2_0(\mathbb{N}\times\mathbb{Z})$.

Lemma 2. *The following facts for the matrix elements $v^{m,0}_{n,n'}$ of the Coulomb potential $1/|z|$ hold:*

- *For all $m \in \mathbb{Z}$ and $n, n' \in \mathbb{N}_0$*

$$0 \leq v^{m,0}_{n,n'} = v^{|m|,0}_{n,n'}. \tag{14}$$

- *For $m, n, n' \in \mathbb{N}_0$*

$$v^{m,0}_{n,n'} \geq v^{m+1,0}_{n,n'}. \tag{15}$$

Proof. The first claim – including the remarkable positivity of all matrix elements – is immediate from the explicit expression (8).

The second claim, i.e., monotony of the matrix elements in m, follows again from (8), if

$$\frac{\Gamma(k+m+3/2)}{\sqrt{\Gamma(n+m+2)\Gamma(n'+m+1)}} \leq \frac{\Gamma(k+m+1/2)}{\sqrt{\Gamma(n+m+1)\Gamma(n'+m+1)}}$$

for $k \leq n, n'$. This is immediate from the functional equation of the Gamma function. □

Lemma 3. *We have*

$$0 \leq (\phi_{m,n}, V\phi_{m,n'}) \leq (\phi_{0,n}, V\phi_{0,n'}) \tag{16}$$

for $n, n' \in \mathbb{N}_0$ and $m \in \mathbb{Z}$.

Proof. By (15)

$$v^{m,0}_{n,n'} + v^{m,1}_{n,n'} \leq v^{0,0}_{n,n'} + v^{0,1}_{n,n'}$$

for all $m \geq 0$.

For negative m

$$v^{m,0}_{n,n'} + v^{m,1}_{n,n'} \leq v^{-1,0}_{n,n'} + v^{-1,1}_{n,n'}$$

where we use all three claims of Lemma 2. Thus, it suffices to show that

$$v^{-1,0}_{n,n'} + v^{-1,1}_{n,n'} \leq v^{0,0}_{n,n'} + v^{0,1}_{n,n'} \tag{17}$$

By (9) we have $v^{0,1}_{n,n'} = v^{1,0}_{n,n'}$ and $v^{-1,1}_{n,n'} = v^{0,0}_{n+1,n'+1}$. Thus (17) is equivalent to

$$v^{0,0}_{n+1,n'+1} \leq v^{0,0}_{n,n'}. \tag{18}$$

This is shown by induction, first in n' and then in n. □

Corollary 2. *For all $a \in l^2_0(\mathbb{N}_0)$ we have*

$$\inf\{\mathcal{E}_m[a] | a \in l^2_0(\mathbb{N}_0)\} \geq \inf\{\mathcal{E}_0[a] | a \in l^2_0(\mathbb{N}_0)\}$$

and

$$\inf\{(u, w_z u) | u \in \mathfrak{q}_0\} = \inf \mathcal{E}_0[l^2_0(\mathbb{N}_0)].$$

Proof. Since the kinetic energy $\sum_n t^m_{n,n}|a_n|$ is obviously invariant under the substitution $a \to |a|$ and since the potential energy

$$-Z \sum_{n,n'} \overline{a_n} \frac{v^{m,0}_{n,n'} + v^{m,1}_{n,n'}}{2} a_{n'}$$

decreases by the same substitution because of the positivity of the potential matrix elements (Lemma 2, Formula (14)), it suffices to take the infimum over positive sequences $a \in l^2_0(\mathbb{N}_0)$ only. Thus, the desired inequalities follow from the corresponding inequalities of the matrix elements (16). □

4. Proof of the theorem

Proof. (Theorem 1) By Corollary 1 it is enough to study w_Z. By Corollary 2, this is equivalent to show lower boundedness of the quadratic form $\mathcal{E}_0$ on non-negative sequences $a \in l^2(\mathbb{N}_0)$.

At this point we embark on a strategy which goes back to Abel – at least – and which has been introduced in relativistic quantum mechanics by Lieb and Yau [13]); it basically consists of estimating a non-diagonal operator by a diagonal one using the Schwarz inequality suitably. We will apply it to the two potential matrices v^0 and v^1 with matrix elements $v^{0,0}_{n,n'}$ and $v^{0,1}_{n,n'}$ (11). (For the matrix elements we will, from now on, suppress the reference to $m = 0$ as well and write simply

$v^\sigma_{n,n'}$, $\sigma \in \{0,1\}$.) Given any sequence $(g_n)_{n\in\mathbb{N}_0}$ with positive entries this strategy suggests estimating as follows:

$$(a, v^\sigma a) \leq \sum_{n=0}^{\infty} \frac{a_n^2}{g_n} \sum_{n'=0}^{\infty} v^\sigma_{n,n'} g_{n'}, \tag{19}$$

where we use matrix notation on the left and that v^σ is symmetric. (Note that we suppress an index σ with g although g can – and will – depend on σ.)

We start with the case $\sigma = 0$ and obtain

$$\begin{aligned}(a, v^0 a) =& \frac{1}{\pi} \sum_{n,n'=0}^{\infty} a_n a_{n'} \sum_{k=0}^{\min\{n,n'\}} \frac{(k+1)_{-\frac{1}{2}}}{(n-k+\frac{1}{2})_{\frac{1}{2}} (n'-k+\frac{1}{2})_{\frac{1}{2}}} \\ &\leq \frac{1}{\pi} \sum_{n=0}^{\infty} \frac{a_n^2}{g_n} \sum_{k=0}^{n} \frac{(k+1)_{-\frac{1}{2}}}{(n-k+\frac{1}{2})_{\frac{1}{2}}} \sum_{n'=0}^{\infty} \frac{1}{(n'+\frac{1}{2})_{\frac{1}{2}}} g_{n'+k}\end{aligned} \tag{20}$$

using (19) and substituting $n' \to n' + k$. We pick for $\sigma = 0$

$$g_n = \frac{1}{(n+\frac{1}{4})_{\frac{3}{4}}}. \tag{21}$$

This allows to explicitly do the summation in n' and k which gives

$$(a, v^0 a) \leq \frac{\Gamma(\frac{1}{4})^4}{2\pi^2} \sum_{n=0}^{\infty} \frac{\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{1}{4})} a_n^2. \tag{22}$$

We apply Gautschi's inequality (50) for $n \in \mathbb{N}$ and we get

$$\frac{\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{1}{4})} \leq \sqrt{n+\tfrac{3}{4}} < \sqrt{n+1} \tag{23}$$

which is also true for $n = 0$ by inspection. Thus,

$$(a, v^0 a) \leq \frac{\Gamma(\frac{1}{4})^4}{2\pi^2} \sum_{n=0}^{\infty} \sqrt{n+1}\, a_n^2. \tag{24}$$

It remains to treat the case $\sigma = 1$. We use again (19) and obtain

$$\begin{aligned}(a, v^1 a) =& \frac{1}{\pi} \sum_{n,n'=0}^{\infty} \frac{a_n a_{n'}}{\sqrt{(n+1)(n'+1)}} \sum_{k=0}^{\min\{n,n'\}} \frac{(k+1)_{\frac{1}{2}}}{(n-k+\frac{1}{2})_{\frac{1}{2}} (n'-k+\frac{1}{2})_{\frac{1}{2}}} \\ \leq& \frac{1}{\pi} \sum_{n=0}^{\infty} \frac{a_n^2}{g_n \sqrt{n+1}} \sum_{k=0}^{n} \frac{(k+1)_{\frac{1}{2}}}{(n-k+\frac{1}{2})_{\frac{1}{2}}} \sum_{n'=0}^{\infty} \frac{g_{n'+k}}{\sqrt{n'+k+1}(n'+\frac{1}{2})_{\frac{1}{2}}}\end{aligned} \tag{25}$$

substituting $n' \to n' + k$. In this case we pick

$$g_n := \frac{\sqrt{n+1}}{(n+\frac{3}{4})_{\frac{5}{4}}} \tag{26}$$

which again allows for explicit summation in n' and k yielding

$$(a, v^1 a) \leq \frac{32\pi^2}{\Gamma(\frac{1}{4})^4} \sum_{n=0}^{\infty} \frac{\Gamma(n+\frac{5}{4})}{\Gamma(n+\frac{3}{4})} a_n^2. \tag{27}$$

For $n \geq 2$ we have

$$(n-\tfrac{1}{4})^{-1/2} < \frac{\sqrt{n+1}}{n+\frac{1}{4}} \tag{28}$$

By Gautschi's inequality (50) the left hand side majorizes $\Gamma(n+\frac{1}{4})/\Gamma(n+\frac{3}{4})$. Thus, by the Gamma function's functional equation we get

$$\frac{\Gamma(n+\frac{5}{4})}{\Gamma(n+\frac{3}{4})} < \sqrt{n+1}. \tag{29}$$

However, this inequality is also true for $n=0$ and $n=1$ by inspection. Thus,

$$(a, v^1 a) < \frac{32\pi^2}{\Gamma(\frac{1}{4})^4} \sum_{n=0}^{\infty} \sqrt{n+1} a_n^2. \tag{30}$$

Putting all together we have

$$\mathcal{E}_0[a] \geq \sum_{n=0}^{\infty} 2\sqrt{n+1}(1 - Z/Z_c) a_n^2 \geq 0 \tag{31}$$

for $Z \leq Z_c$. Note that the first inequality in (31) is indeed strict unless $a = 0$ because of (29). This shows the positivity of the form and therefore the first part of the theorem.

This shows that

$$(u, v)_{\mathfrak{q}} := \sum_{n\in\mathbb{N}_0,\ m\in\mathbb{Z}} ((u, w_z v) + (u, v)) \tag{32}$$

is a scalar product on $\mathfrak{q}_0$ and $(\psi, \varphi)_{\mathfrak{Q}_0} := (\Phi u, \Phi v)_{\mathfrak{Q}}$ is a scalar product on $\mathfrak{Q}_0$. The completions which we denote by $\mathfrak{q}$ and $\mathfrak{Q}$ are subspaces of $L^2(\mathbb{R}^2)$ and $\mathfrak{H}$ respectively. The quadratic form $(\psi, W_Z \psi)$ naturally extend to $\mathfrak{Q}$ and yields the self-adjoint Hamiltonian B_Z.

For completenes we note that for $Z < Z_c$ Equation (31) shows that the norm $\|\cdot\|_{\mathfrak{q}}$ is equivalent to the "Sobolev" type norm $\|u\|_{W_0} := \sum_{m,n} (\sqrt{n+m_+}+1)|(\phi_{m,n}, u)|^2$.

To prove the claimed unboundedness we pick a family of trial sequences a depending on an integer $N \in \mathbb{N}$ – for readability we refrain from indicating this explicitly – given by

$$a_n := \begin{cases} (n+1)^{-3/4} & \text{if } n \leq N \\ 0 & \text{if } n > N. \end{cases} \tag{33}$$

We compute the expectation of the two summands v^σ, $\sigma \in \{0, 1\}$, of the potential energy and obtain

$$\begin{aligned} (a, v^\sigma a) =& \frac{1}{\pi} \sum_{k=0}^{N} (k+\sigma+1)_{-\frac{1}{2}} \left(\sum_{n=1}^{N-k+1} \frac{(n)_{-\frac{1}{2}}}{(n+k)^{\frac{3}{4}+\frac{\sigma}{2}}} \right)^2 \\ =& \frac{1}{\pi} \sum_{k=1}^{N} (k+\sigma+1)_{-\frac{1}{2}} \left(\int_0^{\infty} \frac{\mathrm{d}n}{(n+k)^{\frac{3}{4}+\frac{\sigma}{2}} n^{\frac{1}{2}}} \right)^2 + O(N^0) \\ =& (\tfrac{3}{4}+\tfrac{\sigma}{2})^2_{-\frac{1}{2}} \log(N) + O(N^0) \end{aligned} \tag{34}$$

for large N. Thus

$$\mathcal{E}_0[a] = (a, ta) - Z(a, \frac{v^0+v^1}{2} a) = 2(1 - Z/Z_c)\log(N) + O(N^0), \tag{35}$$

i.e., the form is unbounded from below for $Z > Z_c$. □

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Appendix A. Useful Facts on the Weyl Operator with Homogeneous Magnetic Field

For the convenience of the reader and for fixing the notation we collect in this appendix some facts related to the Weyl operator W_0 with homogeneous magnetic field.

We write $L_n^\alpha(x)$ for the n-th generalized Laguerre polynomial with parameter α (Hochstrasser [12, Formula 22.2.12]). For $m \in \mathbb{Z}$ and $n \in \mathbb{N}_0$ this allows to define the functions

$$\phi_{m,n}(z) = \sqrt{\frac{n!}{\pi(n+|m|)!}} \begin{cases} e^{-\frac{1}{2}z\overline{z}} z^{|m|} L_n^{|m|}(z\overline{z}) & \text{if } m \geq 0 \\ e^{-\frac{1}{2}z\overline{z}} \overline{z}^{|m|} L_n^{|m|}(z\overline{z}) & \text{if } m < 0. \end{cases} \tag{36}$$

In polar coordinates $z = r\exp(\mathrm{i}\varphi)$ these functions are written as

$$\phi_{m,n}(r,\varphi) = \sqrt{\frac{n!}{\pi(n+|m|)!}} e^{-\frac{1}{2}r^2} r^{|m|} L_n^{|m|}(r^2) e^{\mathrm{i}m\varphi} \tag{37}$$

where – in abuse of notation – we use the same notation despite the change of coordinates. Note that these functions form an orthonormal basis of $L^2(\mathbb{R}^2)$ which follows from the fact the $(2\pi)^{-1/2}\exp(\mathrm{i}m\varphi)$ are an orthonormal basis of $L^2(0,2\pi)$ and for every fixed $m \in \mathbb{N}_0$ the generalized Laguerre polynomials L_n^m, $n \in \mathbb{N}_0$, under suitable renormalization, are an orthonormal basis of $L^2((0,\infty), r^m e^{-r}\mathrm{d}r)$ (Hewitt [11]).

Using the recursion relations [12, 22.7.29-32] of the generalized Laguerre polynomials L_n^m and $L_n^{m\prime}(x) = -L_{n-1}^{m+1}$ which is immediate from the definition, we have

$$d^*\phi_{m,n} = 2\mathrm{i}\,\mathrm{sgn}(m)\sqrt{n+m_+ +1}\,\phi_{m+1,n+\theta(-m)} \tag{38}$$

$$d\phi_{m,n} = -2\mathrm{i}\,\mathrm{sgn}(m-1)\sqrt{n+m_+}\,\phi_{m-1,n-\theta(-(m-1))} \tag{39}$$

$$dd^*\phi_{m,n} = 4(n+m_+ +1)\phi_{m,n} \tag{40}$$

$$d^*|d^*|^{-1}\phi_{m,n} = \mathrm{i}\,\mathrm{sgn}(m)\phi_{m+1,n+\theta(-m)} \tag{41}$$

for $n \in \mathbb{N}$, $m \in \mathbb{Z}$, where – as usual – $m_+ := \max\{0,m\}$,

$$\theta(x) := \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases} \text{ and } \mathrm{sgn}(x) := \begin{cases} 1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0 \end{cases}$$

(see also [20, Section 7.1.3]). Note that this solution is related to the non-relativistic Schrödinger equation with homogeneous magnetic field in two dimensions (Fock [7]).

The angular momentum operator L is given as

$$L := x_1 p_2 - x_2 p_1 = z\partial - \bar{z}\bar{\partial} = \frac{1}{\mathrm{i}}\partial_\varphi. \tag{42}$$

Writing the $\phi_{m,n}$ in spherical coordinates easily shows that they are eigenfunctions of L with eigenvalue m, i.e.,

$$L\phi_{m,n} = m\phi_{m,n}. \tag{43}$$

Since the $\phi_{m,n}$ form an orthonormal basis, the eigenvalue equation (45) implies that $|d^*|$ is invertible and $d^*|d^*|^{-1}$ is an isometric operator. The spinors

$$\psi_{m,n} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_{m,n} \\ d^*|d^*|^{-1}\phi_{m,n} \end{pmatrix} \tag{44}$$

for $n \in \mathbb{N}_0$ and $m \in \mathbb{Z}$ form an orthonormal basis of $\mathfrak{H}$ as shown in the proof of Lemma 1.

Using (38) through (41) we find

$$W_0\psi_{m,n} = 2\sqrt{n+m_+ +1}\,\psi_{m,n},\ n \in \mathbb{N},\ m \in \mathbb{Z}, \tag{45}$$

i.e, for fixed $m \in \mathbb{Z}$, the spinor $\psi_{m,n}$ is the n-th eigenvector of W_0 on the positive spectral subspace $\mathfrak{H}$.

The total angular momentum operator J on $L^2(\mathbb{R}^2)$ is given as

$$J = L + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{46}$$

The Formulae (41), (43), and (44) imply

$$J\psi_{m,n} = (m + 1/2)\psi_{m,n}. \tag{47}$$

In fact,

$$[W_0, J] = 0 \text{ and } [w_0, L] = 0. \tag{48}$$

Eventually note, that $\Phi^* J \Phi = L + 1/2$ where Φ is the unitary map defined Lemma 1. This is the reason why it is equally natural to label the basis by the orbital angular momentum quantum number m as to label it by the total angular momentum quantum. We choose m since the formulae are easier to handle.

Appendix B. Some Useful Facts on Gamma and Related Functions

The Gamma function

$$\Gamma(z) := \int_0^\infty z^t e^{-t} \frac{\mathrm{d}t}{t}$$

is obviously positive on the positive half axis $\mathbb{R}_+$ where it is also analytic and log-convex (see, e.g., Rudin [16, Theorem 8.18]).

A useful combination of Gamma functions is the Pochhammer symbol

$$(z)_a := \frac{\Gamma(z+a)}{\Gamma(z)} \tag{49}$$

which is a meromorphic function in both variables z and a.

Lemma 4 (Gautschi [10, Formulae 6 and 7])**.** *For $x \in \mathbb{R}_+$ and $0 \leq s \leq 1$*

$$(x+1)^{s-1} \leq \frac{\Gamma(x+s)}{\Gamma(x+1)} < x^{s-1}. \tag{50}$$

Note that Gautschi claims the inequalities for $x \in \mathbb{N}$ only. However, his proof is valid also for $x \in \mathbb{R}_+$.

Furthermore, we note the reflection formula [4, Formula 6.1.17] which states that for $0 < \Re z < 1$

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}. \tag{51}$$

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